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Stretched and Filtered Transport Synthetic Acceleration of S_N Problems. Part 1: Homogeneous Media

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INTRODUCTION

We present a new method for fast transport synthetic acceleration (TSA) of source iterations for S_N problems, using a pure absorber problem “stretched” to have a mean free path comparable to a diffusion length. The resulting scheme is at first glance unstable, with a large negative eigenvalue at high spatial frequencies, but it can be made effective using (i) a low-pass filter, (ii) a Krylov method, or both. The stretched error correction and the filter are implemented with the same spatial discretization as the underlying source iteration, the Explicit Slope (ES) scheme [1]. In this summary (Part I), we describe the acceleration method, summarize results of Fourier analysis, and give test results in homogeneous planar geometry. In the second summary [2], we describe significant additional features in heterogeneous problems.

STRETCHED AND FILTERED TSA (SFTSA)

Let $\phi^{l+\frac{1}{2}}$ be the scalar flux after the l^{th} source iteration to a steady-state planar-geometry transport problem,

$$\begin{aligned} \mu_n \frac{d}{dx} \psi_n^{l+\frac{1}{2}}(x) + \Sigma_t \psi_n^{l+\frac{1}{2}}(x) \\ = \frac{\Sigma_s}{2} \phi^l(x) + \frac{Q(x)}{2}, \end{aligned} \quad (1)$$

where n is the discrete ordinate index. The exact scalar flux error correction, $F(x) = \phi(x) - \phi^l(x) = \sum_{n=1}^N f_n(x) w_n$, is determined by the transport equation driven by the residual,

$$\begin{aligned} \mu_n \frac{d}{dx} f_n(x) + \Sigma_t f_n(x) \\ - \frac{\Sigma_s}{2} \sum_{n'=1}^N f_{n'}(x) w_{n'} \\ = \frac{\Sigma_s}{2} \left[\phi^{l+\frac{1}{2}}(x) - \phi^l(x) \right] \equiv q_r. \end{aligned} \quad (2)$$

Fast approximate solutions to Eq. (2), by diffusion synthetic acceleration (DSA) or transport synthetic acceleration (TSA) [3, 4], may be used directly by setting $\phi^{l+1} = \phi^{l+\frac{1}{2}} + F$, or by “wrapping” a Krylov method around the accelerated scheme [1-6]. For homogeneous-media source iteration problems, the slowest converging modes are low

spatial-frequency modes, which the diffusion approximation to Eq. (2) eliminates very effectively [4].

For any constant $\epsilon > 0$, the following stretching transformation of the data in Eq. (2) leaves the diffusion approximation invariant,

$$\Sigma_t \leftarrow \frac{\Sigma_t}{\epsilon}, \quad \Sigma_a \leftarrow \epsilon \Sigma_a, \quad q_r \leftarrow \epsilon q_r. \quad (3)$$

Hence, we may pick any constant “stretch” ϵ and expect Eqs. (2) and (3) to still eliminate the low frequency error modes. If we choose $\epsilon = \sqrt{\Sigma_t/\Sigma_a} = 1/\sqrt{1-c}$, then the stretched version of Eq. (2) is given by

$$\begin{aligned} \mu_n \frac{d}{dx} f_n(x) + \Sigma_t \sqrt{1-c} f_n(x) \\ = \frac{\Sigma_t}{2\sqrt{1-c}} \left[\phi^{l+\frac{1}{2}}(x) - \phi^l(x) \right], \end{aligned} \quad (4)$$

which is a pure absorber problem with mean free path $1/(\Sigma_t \sqrt{1-c}) = 1/\sqrt{\Sigma_t \Sigma_a} = \sqrt{3}L$, where L is a diffusion length. We use an S_2 quadrature set for Eq. (4), so that the cost is less than that of a source iteration sweep with quadrature order $N > 2$. Also, since the diffusion Marshak vacuum boundary condition is not invariant to the stretching transformation, we use an albedo boundary condition for Eq. (4) whenever the corresponding boundary condition for Eq. (2) is a vacuum. The albedo boundary condition at $x = 0$ that leaves the stretched boundary condition equivalent to an unstretched Marshak boundary condition (in the P_1 approximation) is given for $\mu_n = -\mu_m > 0$ by

$$f_n = \frac{1-\epsilon}{1+\epsilon} f_m = \frac{\sqrt{1-c}-1}{\sqrt{1-c}+1} f_m.$$

This transformation is important for stability in homogeneous media problems.

An infinite medium Fourier analysis of this approach with the ES spatial discretization [1] gives the $\alpha = 0$ plot in Figure 1a for $\Sigma_t h = 1$ and $c = 0.9999$, and similar plots for other cell thicknesses and scattering ratios. As is evident, the low frequency error modes are effectively eliminated, but the high frequency modes are unstable with a

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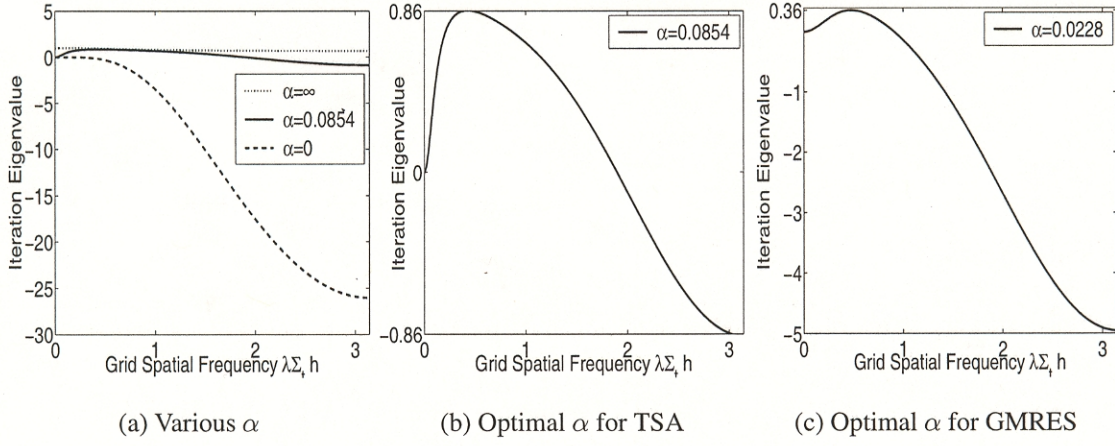


Figure 1: Stretched Filtered TSA Fourier Eigenvalues for $\Sigma_t h = 1$, $c = 0.9999$.

negative eigenvalue. To stabilize the correction, we apply the low-pass filter

$$\begin{aligned} \pm \alpha \frac{d}{dx} g_{\pm}(x) + \Sigma_t \sqrt{1-c} g_{\pm}(x) \\ = \frac{\Sigma_t \sqrt{1-c}}{2} F(x), \end{aligned} \quad (5)$$

where α is the filter strength, to obtain the updated scalar flux

$$\phi^{l+1}(x) = \phi^{l+\frac{1}{2}}(x) + g_+(x) + g_-(x). \quad (6)$$

The filter boundary conditions for Eq. (5) match those of Eq. (2), not those of Eq. (4). This is also important for stability.

The effect of α is demonstrated in Figure 1 for a specific $\Sigma_t h$ and c . Raising α monotonically damps the high-frequency instability but eventually drives the correction to zero and restores unaccelerated source iteration as $\alpha \rightarrow \infty$. The spectral radius of the resulting Stretched, Filtered, Transport Synthetic Acceleration (SFTSA) scheme [Eqs. (1), (4), (5), and (6)] is given by either the maximum positive eigenvalue or the maximum negative eigenvalue, depending on whether α is large or small, respectively. For given values of $\Sigma_t h$ and c , a filter strength α can be calculated, using the Fourier analysis, that minimizes the spectral radius (the maximum positive eigenvalue equals the maximum negative eigenvalue), as demonstrated in Figure 1b. For optimum performance in restarted GMRES, it is desirable for the maximum positive eigenvalue to be a finite distance less than unity, while minimizing the difference between minimum and maximum eigenvalues [1, 5, 6]. Negative eigenvalues < -1 are allowed. By experimentation, we found that by using values of α that maintain the maximum positive eigenvalue less than ≈ 0.36 while minimizing the spread, as in Figure

1c, we obtain nearly optimal performance (as compared to other values of α) when restarted GMRES is “wrapped” around the SFTSA scheme.

NUMERICAL RESULTS

We have implemented SFTSA with the ES spatial discretization [1] in a Fortran test code that can perform SFTSA alone, or SFTSA preconditioned Krylov iteration [1]. Our numerical tests validate the Fourier analysis. In Table 1, we show selected results for two 10,000 cell S_{16} test problems with vacuum boundaries, a uniform volume source $Q = 0.01$, and $\Sigma_t h$ and c as indicated. In the tabulated results, we divide total run times by the time to run a single source iteration sweep. We compare SFTSA (labelled SFT) using the α that optimizes spectral radius as in Figure 1b (precomputed and looked up in a table) to (i) unpreconditioned GMRES (restarted GMRES with maximum subspace dimension 20, labelled G), (ii) SFTSA preconditioned GMRES using α optimized as in Figure 1c, and (iii) SFTSA preconditioned GMRES using $\alpha = 0.3$ fixed. The fixed $\alpha = 0.3$ is greater than nearly all values of α in the optimal table, and hence overfilters most rows in Table 1. We also compare to a DSA calculation, which represents the ideal. Our convergence criterion of 10^{-8} residual norm means that source iteration alone would take roughly 180,000 iterations to converge Problem A and 1800 iterations to solve Problem B.

CONCLUSIONS

Though not as effective as DSA in this one-dimensional setting, SFTSA is nonetheless an effective acceleration strategy. Since the error cor-

Table 1: Numerical Results: CPU Time Relative to a Single Source Iteration Sweep

	$\Sigma_t h$	SFT (α_{opt})	G	G-SFT (α_{opt})	G-SFT ($\alpha = 0.3$)	DSA
Prob. A $c = 0.9999$	0.1	19	4400	16	33	10
	1	84	1477	29	54	11
	10	59	90	24	29	7
	100	12	10	11	11	6
Prob. B $c = 0.99$	0.1	16	105	13	25	11
	1	18	54	14	20	13
	10	10	12	10	10	8
	100	7	5	7	8	5

rection and filter equations, Eqs. (4) and (5), are pure absorber problems, they are as cheap to solve as a source iteration sweep. For idealized homogeneous media problems, a specific filter strength can be derived by Fourier analysis to achieve optimal performance. With the Krylov method “wrapped” around SFTSA, there is less sensitivity to the filter strength, and reasonable efficiency is achieved with a fixed filter strength, $\alpha = 0.3$. This is important for heterogeneous problems, as explained in Part II [2].

SFTSA uses the same spatial discretization as the underlying source iteration scheme. This is one significant advantage of SFTSA over DSA, for which the spatial discretization must be derived from the source iteration scheme with special care. In our DSA results in Table 1, we used a tri-diagonal solver for the diffusion solution at each iteration. In multi-dimensional problems, the diffusion solution in DSA requires a separate iterative solution method. The pure absorber stretch and filter steps of SFTSA, in contrast, are each solved in less time than it takes to conduct a single source iteration sweep. These two advantages make SFTSA an attractive alternative to DSA for complex spatial discretizations and grids.

REFERENCES

- [1] H.L. HANSHAW and E.W. LARSEN, “The Explicit Slope S_N Discretization Method,” *Nuclear Mathematical and Computational Sciences: A Century in Review, A Century Anew*, Gatlinburg TN (2003).
- [2] H.L. HANSHAW, P.F. NOWAK, and E.W. LARSEN, “Stretched and Filtered Transport Synthetic Acceleration of S_N Problems. Part 2: Heterogeneous Media,” *Trans. Am. Nucl. Soc.*, **89** (2003).
- [3] G.L. RAMONE, M.L. ADAMS, and P.F. NOWAK, “A Transport Synthetic Acceleration Method for Transport Iterations,” *Nucl. Sci. Eng.*, **125**, 257 (1997).
- [4] M.L. ADAMS and E.W. LARSEN, “Fast Iterative Methods for Discrete-Ordinates Particle Transport Calculations,” *Prog. Nucl. Energy*, **40**, 3 (2002).
- [5] J.S. WARSA, T.A. WAREING, and J.E. MOREL, “Krylov Iterative Methods Applied to Multidimensional S_N Calculations in the Presence of Material Discontinuities,” *Nuclear Mathematical and Computational Sciences: A Century in Review, A Century Anew*, Gatlinburg TN (2003).
- [6] Y. SAAD, *Iterative Methods for Sparse Linear Systems, Second Edition*, SIAM (2003).

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